Spermine, tetrakis-MOC derivative

Inchi: InChI=1S/C16H32N4O6/c1-24-14(21)18-10-6-9-17-8-4-5-12-20(16(23)26-3)13-7-11-19-1
InchiKey: QZHZSQNMWZRHNY-UHFFFAOYSA-N
Formula: C16H32N4O6
SMILES: COC(=O)NCCCNCCCCN(CCCNC(=O)OC)C(=O)OC
Mol. weight [g/mol]: 376.45

Physical Properties

Property code	Value	Unit	Source
gf	-238.97	kJ/mol	Joback Method
hf	-880.03	kJ/mol	Joback Method
hfus	63.87	kJ/mol	Joback Method
hvap	100.03	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	0.917		Crippen Method
mcvol	298.540	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	3055.00		NIST Webbook
tb	957.30	K	Joback Method
tc	1172.50	K	Joback Method
tf	677.01	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.49	J/mol×K	957.30	Joback Method
cpg	1013.69	J/mol×K	993.17	Joback Method
cpg	1025.47	J/mol×K	1029.03	Joback Method
cpg	1035.87	J/mol×K	1064.90	Joback Method
cpg	1044.88	J/mol×K	1100.77	Joback Method
cpg	1052.54	J/mol×K	1136.63	Joback Method
cpg	1058.85	J/mol×K	1172.50	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333747&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume